

Statistical mechanics of exploding phase spaces

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Real complex systems, as encountered in biology or neuroscience, typically involve components that interact and create new emergent states leading to phase spaces whose volumes grow super-exponentially (“exploding”) with the number of degrees of freedom. We argue that the standard ensemble theory could break down for such cases and illustrate this phenomenon using simple models. We present a rigorously defined entropy which is extensive in the micro canonical, equal probability, ensemble for super-exponentially growing phase spaces. We suggest that this entropy may be useful in determining probability measures for such systems through appropriately constrained maximum entropy procedures.

The methodology of statistical physics as established by Gibbs and Boltzmann and others around 1900 derives macroscopic properties from the behaviour of the microscopic components by assigning probabilistic weights to the micro states constituting the phase space of the system [1]. Can this approach be expanded in ways that makes it possible to analyse systems typically considered by complexity science, such as ecology, biology, neuronal dynamics, economics etc. [2–4]? This generalization necessitates that we establish how in general to handle phase spaces and their probability measures for complex systems. One line of research suggests that ergodicity breaking and strong restrictions on the available phase space volume is of particular relevance to complex systems [5, 6]. This may appear plausible when one considers situations, as typical in physics, where the set of all possible states of a macroscopic system consists of subsets of the direct product of the states the individual components can occupy. The situation is different when one, instead of thinking of degrees of freedom characterizing “particles”, consider the functionality of the macrosystem and how these relate the components. Especially evolutionary biologist have for sometime discussed this. Stuart Kauffman [7] points out: *Because these evolutionary processes typically cannot be pre-stated, the very phase space of biological, economic, cultural, legal evolution keeps changing in unpre-statable ways. In physics we can always pre-state the phase space, hence can write laws of motion, hence can integrate them to obtain the entailed becoming of the physical system.* Similar difficulties are pointed out by Nors Nielsen and Ulanowicz[8] in their discussion of ontic openness, or combinatorial explosion, encountered in developmental biological processes. This suggests that the size of the configuration spaces for complex systems, such as those encountered in biology, grow super-exponentially. We will here concern ourself with the consequences for statistical mechanics (in the sense of a static treatment of the mechanisms underlying the

macroscopic behavior) when new paired states are created and the phase space volume as a consequence grows faster than the direct product k^N of the combination of single N component states each being able to occupy k different states.

For a concrete simple example of the above, consider the chemical activation energy for two chemical species with constant number of molecules, kept at constant temperature. At sufficiently low temperature the activation energy may act as an unsurmountable energy barrier so the system remains in equilibrium with no reaction between the two chemicals. Next assume the existence of an enzyme that facilitates the chemical reaction between the species and thereby move the system to a new thermodynamic state with a new composition. Adding the enzyme will accordingly move the system to a new equilibrium. In this way we see that the two chemical species plus the enzyme introduce a new paired state, and a bigger phase space, than the one related to the two chemical species plus adding a molecule with no effect on the chemical reaction.

Having realised that complex systems often exhibit exceptional growth rates of their available phase space volume as function of number of degrees of freedom, one may ask if applying the standard formalism of statistical mechanics, *i.e.* micro canonical or canonical ensemble theory, will flag up warnings signs in terms of inconsistencies?

The following simple example suggests that super-exponential phase space growth may lead to problems. We assume for a moment that the ordinary thermodynamical description remains unaltered and consider a grand canonical system consisting of N particles. Our line of thinking is not dissimilar to the one followed by Kosterlitz and Thouless [9] in their seminal analysis of the vortex unbinding transition in the 2 dimensional XY-model. To represent the emergence of composite structures and the related super-exponential phase space we

assume that the N particles can occupy $W(N) = N^N$ states and that each of these states have the energy $E = NE_0$. The (grand canonical) free energy of the system is accordingly given by

$$F = N[E_0 - k_B T \log N - \mu]. \quad (1)$$

where k_B denotes Boltzmann's constant, T is the temperature and μ the chemical potential. This expression implies that the system can gain free energy by absorbing new degrees of freedom, $dF/dN < 0$, when $N > \exp((E_0 - \mu)/k_B T - 1)$. This suggests that exploding phase space volumes can cause problems for the standard theory. Next we investigate the situation in more detail.

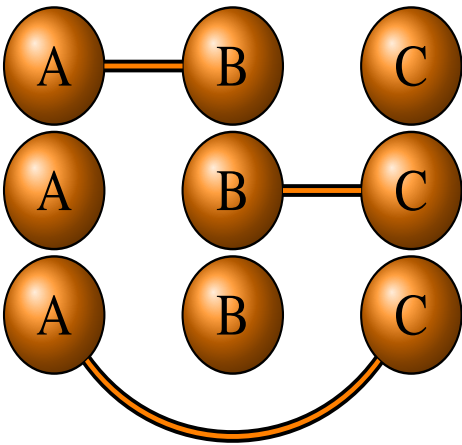


Figure 1. We assume all pairs are distinguishable. Hence we consider all the possible pairings between $2p$ elements which is $(2p - 1)!!$ combinations. This is shown in following figure for three coins and one pair.

To set the scene we consider the following “Magnetic Coin Model”, which consists of N coins in various configurations. If each coin shows either heads or tails, the (discrete) available phase space grows like $W(N) = 2^N$, resembling that of the Ising Model. *Instead* of being oriented, for $N > 1$ we may also allow for a paired state, with two coins sticking to each other. Fig. 1 illustrates the pairing. Adding a single coin doubles the phase space, $2W(N)$, due to the coin's orientation (heads or tails). In addition the new magnetic coin can be paired with any of the N coins in the aggregate (which leaves $W(N - 1)$ states for the remaining coins), so there exist $NW(N - 1)$ possible states for the second case. In total

$$W(N + 1) = 2W(N) + NW(N - 1). \quad (2)$$

The power series generating function for this recursive relation is $G(x) = \exp(2x) \exp(\frac{x^2}{2})$ with $G(x) =$

$\sum_n W(n) \frac{x^n}{n!}$. For even N the exact solution is

$$W(N) = \sum_{k=0}^{N/2} \frac{N! 2^{3k-N/2}}{(2k)!(N/2 - k)!}, \quad (3)$$

which asymptotically for $N \gg 1$ behaves like

$$W(N) = \frac{1}{\sqrt{2e}} \left(\frac{N}{e}\right)^{N/2} e^{2\sqrt{N}} \left(1 + O\left(\frac{1}{\sqrt{N}}\right)\right). \quad (4)$$

We conclude that the number of states grows faster than exponentials and slower than factorials. Analogous formulas hold for N odd.

As illustrated by the Magnetic Coin Model, explosive (*i.e.* super-exponentially growing) phase spaces are easily obtained by allowing the constituent N parts to *relate* to each other. We believe this situation is generic and mention here a couple of examples: one from game theory and two from network theory. For example the space of strategies to consider on the basis of a history of length N of either defecting or cooperating, is $2^{(2^N)}$, namely either defect or cooperate for every possible history of length N , of which there are 2^N . Less dramatically increasing, but still explosive, is the space of $2^{(N^2)}$ general directed adjacency matrices, allowing one directed edge between any (not necessarily distinct) two of N nodes.

Our third example consist in restricting adjacencies to those where each node has out-degree of exactly 1, *i.e.* each of N nodes has exactly one edge to any of N nodes, produces a phase space volume of $W(N) = N^N$, logarithmically with the same leading N dependence of $W(N)$ as for the Coin Model in Eq. (4).

Let us turn to the entropy. The faster than exponential N dependence of $W(N)$ will cause the Boltzmann entropy $S = k_B \log W(N)$, for the equal probability micro canonical ensemble, to grow faster than linearly. We will refer to an entropy as being “extensive” if the limit $\lim_{N \rightarrow \infty} \frac{S(N)}{N} = \text{constant} < \infty$. Therefore Boltzmann's entropy in our case isn't extensive. We will below introduce an extensive entropy, but first we consider briefly the Magnetic Coin Model in the canonical ensemble.

To make contact to the canonical ensemble we introduce the following Hamiltonian

$$\mathcal{H} = -B \sum_{i=1}^N \sigma_i, \quad (5)$$

where states of the systems are parametrised according to

$$\sigma_i \in \{-1, 0, 1\}, \quad (6)$$

corresponding to coins in down, paired and up states respectively in an external field B . Since paired coins do not contribute to the energy the Hamiltonian reduces to $\mathcal{H} = -B \sum_{\{\sigma_i\}} \sigma_i$, where $\{\sigma_i\}$ is the set of coins that

are not in pair state. As a result the partition function is calculated by counting all the configurations that contain the same number of pairs p and weigh this number by the Boltzmann factor $Z_{N,p} = e^{-\beta\mathcal{H}}$ and then sum over p .

$$Z(N, \beta) = \sum_{p=0}^{\frac{N}{2}} (2p-1)!! \binom{N}{2p} Z_{N-2p} = \sum_{p=0}^{\frac{N}{2}} 2^{N-2p} (2p-1)!! \binom{N}{2p} \cosh^{N-2p}(\beta B). \quad (7)$$

From this expression we can compute the free energy and obtain

$$F(\beta) = \lim_{N \rightarrow \infty} \frac{1}{N} \log \left(\sum_{p=0}^{\frac{N}{2}} t_{N,p} \right) \rightarrow \infty. \quad (8)$$

Here

$$t_{N,2p} = 2^{N-2p} (2p-1)!! \binom{N}{2p} \cosh^{N-2p}(\beta B). \quad (9)$$

We conclude that the free energy is non-extensive. A remark about distinguishability is pertinent. As is usually the case when dealing with the Ising model, we consider the coins to be distinguishable. However, if, when the pairing is considered, the coins are considered to be indistinguishable the resulting free energy becomes extensive. This is not to be confused by the usual Gibbs' paradox, as for example discussed by Janyes [10]. Rather we consider the situation for the Magnetic Coins to be similar to the usual Ising model, where the individual spins, or coins in our case, are considered to be distinguishable by, say, their fixed position in some lattice structure.

Next we establish an entropy which is extensive for exploding phase space volumes. We will construct an entropy which adheres to the first three Shannon-Khinchin axioms (see e.g. [11] and Appendix A of [12]), replacing the fourth on additivity by a generalised composability. We suggest that such an entropy may help to establish a statistical mechanics for exploding phase spaces. We consider the Z-Entropies recently introduced by one of the authors [12, 13].

Ref. [12] explains how one in general can derive an axiomatically rigorous entropy that is extensive for a give phase space growth rate. For this procedure to be tractable in a fully exact manner the inverse of the growth rate has to be given in a closed form. We cannot do this for the phase space growth rate given in Eq. (4) for the Magnetic Coin model, we therefore restrict ourselves to the stringest N dependence of Eq. (4) and consider

$$W(N) \sim N^{\gamma N}, \quad (10)$$

where γ is a positive real parameter. We look for a group entropy which is extensive on a phase space growing according to the rate function (10). We first define a general entropy, valid for any phase space growth rate, and then we show that it is extensive when $W = W(N)$ is given by eq. (10).

Let $\{p_i\}_{i=1, \dots, W}$, $W \geq 1$, with $\sum_{i=1}^W p_i = 1$, be a discrete probability distribution. We introduce the entropy

$$S_{\gamma, \alpha}[p] := \exp \left[L \left(\frac{\ln \sum_{i=1}^W p_i^\alpha}{\gamma(1-\alpha)} \right) \right] - 1 \quad (11)$$

where $0 < \alpha < 1$, $\gamma > 0$.

Here we denote by $L(x)$ the Lambert function $W_0(x)$, which is a single-valued and invertible function

The entropy $S_{\gamma, \alpha}$ is extensive, over the uniform distribution, for the phase space growth rate $W(N) \sim N^{\gamma N}$.

Suppose $p_i = 1/W$, $i = 1, \dots, W$. We have

$$\begin{aligned} S_{\gamma, \alpha}[W(N)] &= \exp \left[L \left(\frac{\ln W(N)^{1-\alpha}}{\gamma(1-\alpha)} \right) \right] - 1 \\ &= \exp \left[L \left(\frac{\ln W(N)}{\gamma} \right) \right] - 1. \end{aligned} \quad (12)$$

Now, since eq. (10) holds, we have

$$S_{\alpha; N} = \exp [L(N \ln N)] - 1 = N - 1, \quad (13)$$

where we took into account the property

$$L(N \ln N) = \ln N.$$

Consequently,

$$\lim_{N \rightarrow \infty} \frac{S(N)}{N} = \text{const},$$

which proves extensivity. Next we observe that the entropy (11) satisfies the SK axioms.

(SK1) (Continuity). The function $S_{\gamma, \alpha}(p_1, \dots, p_W)$ is continuous with respect to all its arguments

(SK2) (Maximum principle). The function $S_{\gamma, \alpha}(p_1, \dots, p_W)$ takes its maximum value on the uniform distribution $p_i = 1/W$, $i = 1, \dots, W$.

(SK3) (Expansibility). The entropy stays invariant if we add an event of zero probability: $S_{\gamma, \alpha}(p_1, \dots, p_W, 0) = S_{\gamma, \alpha}(p_1, \dots, p_W)$.

The entropy (11) is non-additive [14]-[15]. However, it satisfies a generalization of the SK fourth axiom: the composability axiom.

The precise definition of composability was introduced in [13], [12]: An entropy S is strongly (or strictly) *composable* if there exists a smooth function of two real variables $\Phi(x, y)$ such that

$$(C1) \quad S(A \cup B) = \Phi(S(A), S(B); \{\eta\}) \quad (14)$$

where $A \subset X$ and $B \subset X$ are two statistically independent subsystems of a given system X , defined for any probability distribution $\{p_i\}_{i=1}^W$, $\{\eta\}$ is a possible set of real continuous parameters, with the further properties

(C2) Symmetry:

$$\Phi(x, y) = \Phi(y, x). \quad (15)$$

(C3) Associativity:

$$\Phi(x, \Phi(y, z)) = \Phi(\Phi(x, y), z). \quad (16)$$

(C4) Null-composability:

$$\Phi(x, 0) = x. \quad (17)$$

The entropy $S_{\gamma, \alpha}$ is *composable*.

Let

$$G(t) = (1 - \alpha) \left\{ \exp \left[L \left(\frac{t}{1 - \alpha} \right) \right] - 1 \right\}.$$

The generalized logarithm associated with $G(t)$ is

$$\ln_G(x) := G(\ln x).$$

Then the entropy (11) can be written in the form

$$S_{\gamma, \alpha}[p] = \frac{\ln_G \left(\sum_{i=1}^W p_i^\alpha \right)}{1 - \alpha}, \quad (18)$$

i.e. it is a representative of the Z -class of entropies introduced in [12].

According to the theory of formal groups [16], [17], [18], the group law associated with the entropy (11) is given by the general expression

$$\Phi(x, y) = G(G^{-1}(x) + G^{-1}(y)). \quad (19)$$

Precisely, we have

$$\Phi(x, y) = \exp [L((1+x)\ln(1+x) + (1+y)\ln(1+y))] - 1. \quad (20)$$

One can prove directly that the function $\Phi(x, y)$ satisfies the properties (C2)–(C4).

We can conclude that $S_{\gamma, \alpha}$, being strictly composable and satisfying the first three SK axioms, belongs to the class of *group entropies* [19], [12], [13]. In addition to being an entropy in this axiomatic sense, it is also worth pointing out that the group structure ensures that an additive information measure is associated with our entropy. This measure is given by

$$I(A) = \psi^{-1}(Z(A)). \quad (21)$$

We get immediately that $I(A) = \frac{1}{1-\alpha} \ln \left(\sum_{i=1}^W p_i^\alpha \right)$, i.e. it coincides with the celebrated Rényi entropy [20].

Finally we note that our discussion of the case $W(N) = N^{\gamma N}$ is also relevant to the Magnetic Coin model. For the entropy in Eq. (13) the factor $\exp(2\sqrt{N})$ in Eq. (4) will be irrelevant compared to the factor $N^{N/2}$ since $S_{\alpha; N}$ depends on $W(N)$ through $\ln(W(N))$. In both cases $\lim_{N \rightarrow \infty} S_{\alpha; N}/N = \gamma$, with $\gamma = 1/2$ for $W(N)$ in Eq. (4).

Let us summarise that we have presented a functional on the space of probability measures on configuration space, which has the properties of an entropy in the sense of the first three Shannon-Khinchin axiom plus it possesses the property of composability as described in (C1-C4) above. This entropy is extensive in the equal probability micro canonical ensemble. The question then arises, how we establish the non-uniform probability weights. One may suggest that given the axiomatic properties together with the extensivity, it is possible that this entropy, Eq. (11), can form the basis for a Maximum Entropy procedure as Jaynes describes for the standard case in [21]. One would then derive a generalisation of the canonical ensemble by, say, maximising the entropy corresponding to Eq. (4) under the constraints $\sum_{i=1}^{W(N)} p_i = 1$ and $\sum_{i=1}^{W(N)} \mathcal{E}_i p_i = \langle \mathcal{E} \rangle$ with the energies given by the Hamiltonian in Eq. (5). One formally obtains $p_i = (1 + b\mathcal{E}_i)^{1/(\alpha-1)}/Z$, where Z is a normalisation factor and b is the ratio of the two Lagrange multipliers corresponding to the two constraints. Obviously more work is needed to establish the applicability of this approach.

We find that the axiomatic approach presented above ensures that the foundation of the entropy is transparent and consistent, namely that axioms (SK1-3) and (C1-4) are satisfied, but this foundation only determines the entropy up to the parameter α . The meaning and determination of the α parameter remains to be established. However, we surmise that the determination of α will be related to the specifics of the maximisation procedure.

We end by stressing the importance of super-exponential phase space growth for complex systems in which essential emergence takes place. It is important to find ways to establish a statistical mechanics formalism that is applicable to such situations. We suggest that the entropy introduced here is an interesting candidate.

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